Effect of Γ–X mixing on electron tunneling times in GaAs/AlAs double barrier heterostructures

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The effect of Γ–X mixing on electron tunneling time in GaAs/AlAs symmetric double barrier heterostructures is studied theoretically using an empirical tight-binding band structure model. It is found that the Γ quasibound state tunneling times can be shortened or lengthened by Γ–X mixing, depending on whether the AlAs barriers consist of an even or odd number of monolayers. This is attributed to the interference between the Γ and X conduction channels in the AlAs barriers.

I. INTRODUCTION

Since negative differential resistance (NDR) in the double-barrier heterostructure (DBH) was originally proposed[1] and demonstrated[2] by Chang, Tsu, and Esaki, there has been extensive investigations aimed at understanding the process of resonant tunneling, and at exploiting the electrical properties of DBH for high-speed analog and digital applications. A particularly interesting application of double barrier resonant tunneling diodes has been found in the area high-speed oscillators, which has witnessed steady performance improvement.[3–5] Recently, microwave oscillations up to 712 GHz were reported in double-barrier resonant tunneling diodes.[5] An important characteristic of the double-barrier resonant tunneling diodes in high-speed applications is the tunneling time. Brown *et al.* showed that the maximum attainable oscillation frequency and power output in a resonant tunneling diode is strongly dependent on DBH quasibound state lifetimes. A number of researchers[6,7] have measured tunneling escape times of the lowest quasibound states in GaAs quantum wells (QWs) (hereafter referred to as $\Gamma 1$ states for convenience). These studies examined the barrier-width dependence of the $\Gamma 1$ state tunneling time in structures with relatively wide QWs, reporting times as short as 12 ps.[7] A photoluminescence study[8] of a series of double-barrier structures with varying well width offered indirect evidence that the $\Gamma 1$ state tunneling time in structures with narrow wells may be strongly influenced by Γ–X mixing.

To demonstrate the effect of Γ–X mixing on the tunneling escape of electrons from GaAs wells, we have performed a calculation comparing the dynamics of the tunneling escape processes in wide- and narrow-well GaAs/AlAs double-barrier structures. We use the one-band Wannier orbital model[9] to describe the conduction band structures of GaAs and AlAs, and solve the time-dependent Schrödinger equation to obtain the time evolution of a wave function initially localized in the GaAs QW.[10] The initial wave function is chosen to be constant in the GaAs well, and zero elsewhere; it therefore contains a large $\Gamma 1$ component, plus smaller contributions from the higher lying quasibound states. Since the higher quasibound states have shorter lifetimes, the long term behavior of the wave function reflects the escape process of the $\Gamma 1$ state. Figure 1 shows the time evolution of electron probability densities integrated over the well region and over barrier regions for: (a) a wide-well structure and (b) a narrow-well structure. The insets of Fig. 1 shows the conduction band diagrams, including both the Γ-point and the X-point profiles, and the $\Gamma 1$ levels of the two structures. Note that the X-point profile shows a double QW configuration, which can accommodate quasibound states of its own. In the wide-well case, the $\Gamma 1$ level is sufficiently low in energy and is largely unaffected by the X-point states. But in the narrow-well case, the $\Gamma 1$ level is comparable in energy to the X-point states, and can interact strongly with them. Figure 1(a) shows the tunneling escape process in the wide-well structure. After the rapid escape of the components associated with the higher lying quasibound states, the probability density in the well decays exponentially, with the decay time constant corresponding to the $\Gamma 1$ lifetime. The probability density in the barrier region is relatively small throughout the decay process. In contrast, the narrow-well case in Fig. 1(b) shows the probability density oscillating back and forth between the well and barrier regions during the decay process, indicating strong mixing between the $\Gamma 1$ states localized in the GaAs well region and X-point resonances localized in the AlAs barrier regions.

The striking difference between the tunneling escape processes in the wide- and narrow-well structures suggests that the $\Gamma 1$ state lifetime is strongly dependent on Γ–X mixing. To determine the role of Γ–X mixing, we have performed a theoretical calculation of the lifetimes of quasibound states in GaAs/AlAs double barrier heterostructures. An eight-band second-neighbor sp^3 tight-binding model[11] is used to provide a realistic description of band structures. Quasibound state lifetimes are estimated from the full width at half-maximum (FWHM) of the transmission resonances in the transmission spectra using the uncertainty principle

$$\tau \cong \frac{\hbar}{\Delta E_{\rm FWHM}}. \tag{1}$$

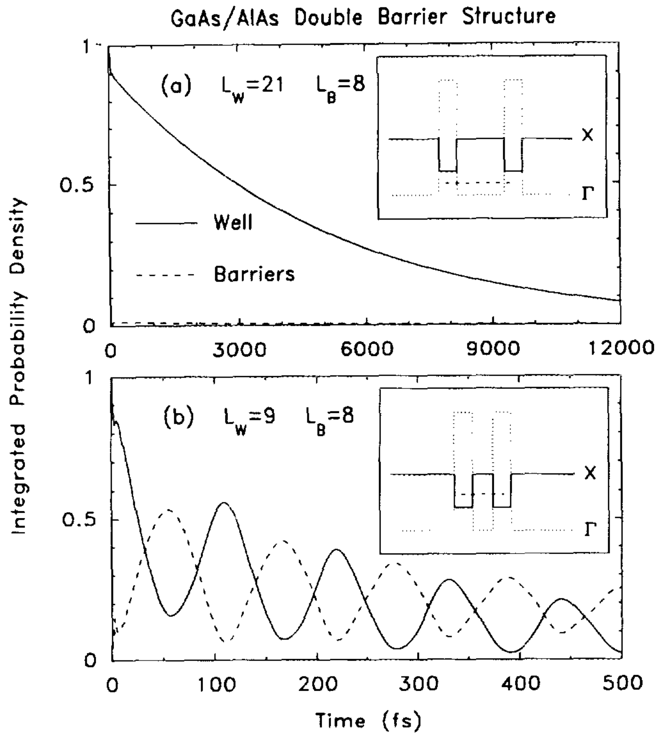

FIG. 1. Time evolution of probability densities integrated over the well (solid curve) and barrier (dashed curve) regions depicting the escape of an electron initially localized in the GaAs well region of a (001) GaAs/AlAs symmetric double-barrier structure. The top panel illustrates the wide-well case (21 ML well, 8 ML barrier) where Γ–X interaction is insignificant, and the bottom panel illustrates the narrow-well case (9 ML well, 8 ML barrier) where the influence of Γ–X mixing can be clearly seen. The insets show the conduction band profiles at the Γ point and the X point for the two structures, with the dashed lines indicating the energy levels of the lowest Γ quasibound states.

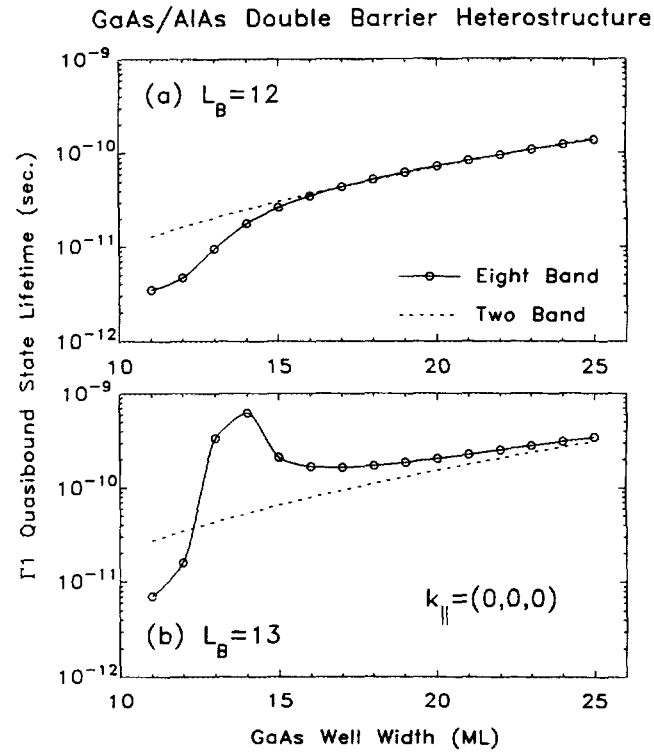

FIG. 2. Tunneling life times for the Γ point $n = 1$, $\mathbf{k}_{\parallel} = 0$ quasibound states in GaAs/AlAs symmetric double-barrier heterostructures, with GaAs well widths ranging from 5 to 25 ML, and AlAs barrier widths of (a) 12, and (b) 13 ML. Results obtained with a simple two-band model are shown as dashed lines for comparison with the eight-band model results.

II. RESULTS AND DISCUSSION

Figure 2(a) shows the lifetimes of the Γ1 resonance as a function of GaAs well width (L_W). The barrier width (L_B) is fixed at 12 monolayers (ML). For reference, we also show the Γ1 state lifetimes predicted by a simple two-band model which only includes the Γ-valley band structure of the lowest conduction band and the light-hole band. The effect of Γ–X mixing on quasibound state tunneling lifetimes can be readily seen by comparing the results from the two models. The two-band model, which does not incorporate Γ–X mixing effects, predicts that the Γ1 resonance lifetime decreases monotonically with GaAs well width. This is as expected, since quasibound states in narrower wells have higher energy, and are less confined. Comparing the eight-band and the two-band curves, we note good agreement in the wide-well limit where Γ–X mixing is insignificant. But as the well width narrows to below 15 ML where Γ–X mixing becomes important, the eight-band curve diverges from the two-band curve, predicting considerably shorter tunneling times. The difference might be interpreted as follows. While purely Γ-like quasibound states are confined largely in the GaAs QW, the Γ–X mixed quasibound states have wave functions which extend significantly into the AlAs layers. Being less confined, the Γ–X quasibound states have shorter lifetimes. The results shown in Fig. 2(a) agrees with what we might expect intuitively, that by supplying additional escape channels, the X-point levels in the AlAs layers enhance the tunneling escape rates of GaAs QW quasibound states.

Although the simple intuitive picture seems to provide a reasonable explanation for Γ–X mixing effects seen in Fig. 2(a), we will demonstrate that it can be quite inadequate in certain instances. In Fig. 2(b) we again show the lifetime of Γ1 resonance in double-barrier structures as a function of the GaAs well width. The structures are identical to those shown in the previous example, except that the AlAs barrier width has been changed from 12 to 13 ML. Here, again, we note reasonable agreement between the eight-band and two-band results in the wide well limit. But as we decrease the GaAs well width, the eight-band curve initially decreases (but more slowly than the two-band curve), and then rises to a maximum at $L_W = 14$ before dropping below the two-band curve for $L_W = 12$ and $L_W = 11$. At $L_W = 14$, the eight-band lifetime exceeds the two-band result by more than an order of magnitude. There are two aspects of this result which are surprising. First, the increase in tunneling times found in Fig. 2(b) clearly contradicts the hypothesis presented earlier that Γ–X mixing should enhance tunneling rates. Moreover, there is a dramatic difference between the tunneling time curves shown in Figs. 2(a) and 2(b), even though the two sets of structures differ only by a single monolayer in barrier width.

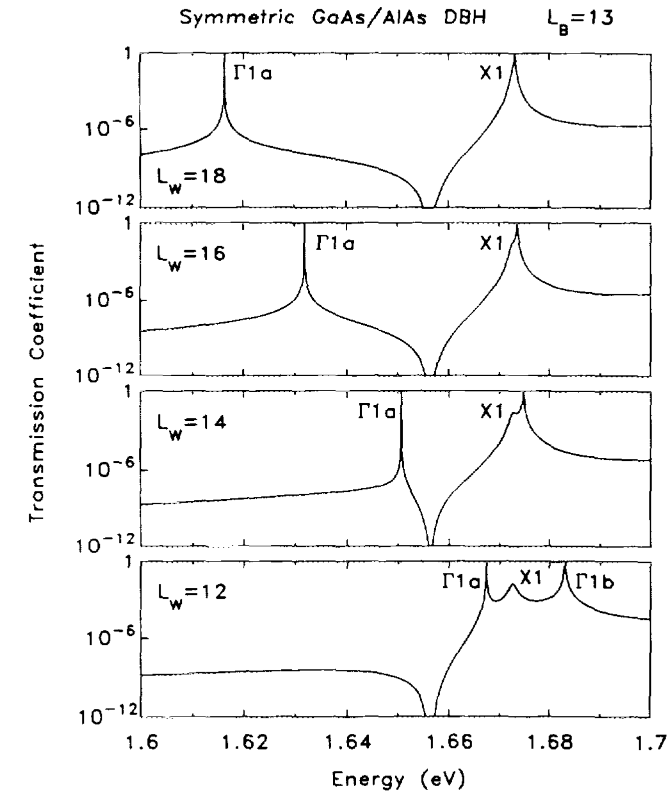

FIG. 3. Transmission coefficients for (001) GaAs/AlAs symmetric double-barrier heterostructures with GaAs well widths of 12, 14, 16, and 18 ML. The width of the AlAs barrier is 13 ML, and $\mathbf{k}_{\parallel}=0$. The width of the Γ1*a* peak is used to calculate the lifetimes shown in Fig. 2(b).

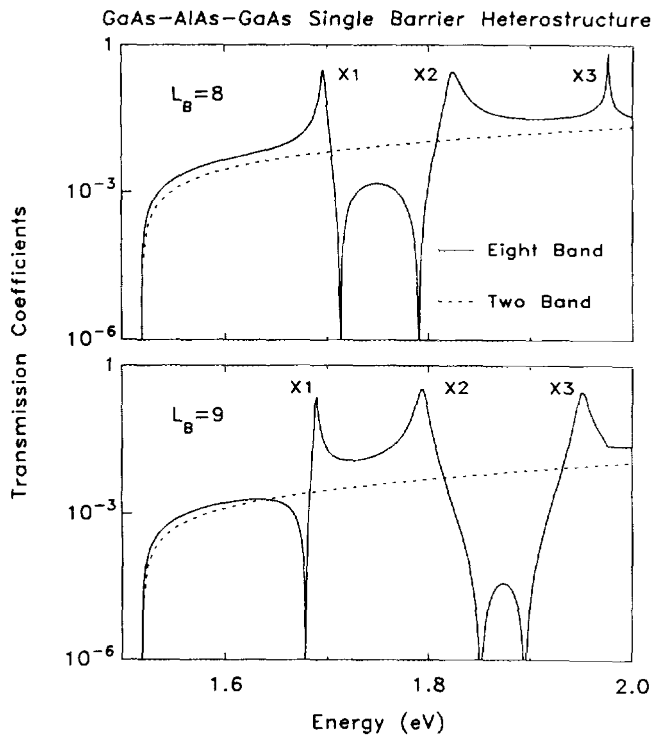

FIG. 4. Transmission coefficients at $\mathbf{k}_{\parallel}=0$ for (001) GaAs/AlAs single-barrier heterostructures with AlAs barrier widths of 8 and 9 ML. Results obtained with eight-band tight-bind model and simple two-band model are shown in solid and dashed lines, respectively.

We first illustrate how the Γ1 resonance lifetime is increased by Γ–X mixing. In Fig. 3 we examine transmission coefficients for a set of double-barrier structures with $L_B=13$. In each plot a dip in the transmission spectrum, known as an antiresonance, is found at $E\approx 1.656$ eV. In contrast to resonances, which give rise to enhanced transmission, the antiresonances impede transmission. A comparison of Fig. 2(b) and Fig. 3 suggests that the Γ1 lifetime increase is caused by the linewidth narrowing in the Γ1 resonance as it approaches the antiresonance. This conjecture is consistent with the observation (not shown) that antiresonances are absent in the transmission spectra of double barrier structures with $L_B=12$, for which no lifetime increase is found.

The sensitivity of antiresonances to variations in the AlAs barrier width and the insensitivity of antiresonance positions to variations in the GaAs welll width (see Fig. 3) indicate that antiresonances are associated with the AlAs X-point QWs rather than the GaAs Γ-point QW. This suggests that we could understand the origin of the antiresonances by focusing on tunneling in the AlAs layers. In Fig. 4 we examine the transmission spectra for GaAs–AlAs–GaAs single barrier structures with $L_B=8$ and $L_B=9$, calculated using the two-band and the eight-band models. The two-band transmission spectra exhibit the conventional single-barrier tunneling behavior, increasing monotonically with energy. The eight-band spectra show resonances and antiresonances due to the presence of the X-point QW. Ko and Inkson[12] suggested that the antiresonances may be understood in terms of Fano resonances,[13] which are formed when discrete levels are coupled to continuum states. A Fano resonance consists of a zero and a pole and is easily recognized by the distinctive asymmetric line shape showing a dip next to the resonance peak. In the GaAs–AlAs–GaAs single-barrier structure, the bound states in the X-point QW interact with the continuum of Γ states to form a set of Fano resonances. The antiresonances seen in our transmission spectra are the X-point Fano resonance dips.

In the example of the $L_B=8$ structure shown in Fig. 4, the $X1$ Fano resonance is seen as a peak followed by a dip in the transmission spectra, while the $X2$ resonance appear as a dip followed by a peak. Comparing the transmission spectra for the $L_B=8$ and the $L_B=9$ structures, we note that the sequence of peaks and dips are reversed in the two cases. A systematic study of transmission spectra for L_B ranging from 3 to 40 reveals opposite peak/dip sequences for structures with odd and even L_B's, with the odd-L_B structures showing leading dips and even-L_B structures showing leading peaks. In fact, for $L_B>10$, resonance peaks are closely spaced, and no antiresonances are found between peaks; thus, the even-L_B structures show no antiresonances at all, and the odd-L_B structures show only the leading $X1$ antiresonances.[14]

Since the lengthening of the Γ1 resonance lifetime in double-barrier structures is caused by the interaction with the leading $X1$ antiresonance, the peculiar L_B dependence of the $X1$ Fano resonance peak/dip ordering is directly responsible for the difference between the Γ1 lifetime curves shown in Figs. 2(a) and 2(b). To account for the L_B dependence of the peak/dip ordering of the $X1$ Fano resonance, we make use of the complex conductance analogy by Ko and Inkson.[12] It was shown that, for tunneling through a barrier with multiple tunneling channels, the coefficient of a transmitted state may be written as[12]

$$t = \sum_j \alpha_j \exp[i(k_j^R + ik_j^I)W] \equiv \sum_j Y_j, \tag{2}$$

where W is the width of the barrier, k_j^R and k_j^I are the real and imaginary parts of the complex wave vector of the jth tunneling state in the barrier, and α_j depends on the scattering properties of the interfaces; the summation is taken over all exponentially decaying and forward propagating states. In analogy to parallel circuits, each tunneling channel can be considered as having a complex conductance of Y_j. As in a parallel circuit, both the magnitudes and the phases of the complex conductances are important in determining the total transmission coefficient. In the AlAs barrier, the Γ and X tunneling states in the energy range of interest have purely imaginary and purely real wave vectors, respectively. Thus, while the Γ-channel phase does not vary with the barrier width, the X-channel phase is barrier-width dependent. To illustrate this dependence, we write a wave vector k in the X valley as $k = k_0^X + (k - k_0^X) \equiv k_0^X + q$, where k_0^X is the wave vector of the X minimum, and q represents the wave vector k measured from the X minimum. This allows us to write the propagation factor $\exp(ikW)$ as the product of a rapidly oscillating term $\exp(ik_0^X W)$, which described the consequence of having the conduction band minimum located away from the zone center, and a slowly varying term $\exp(iqW)$, which determines the resonance condition in the same way that a Γ-valley propagation factor does (i.e., qW plus phase changes at the interfaces must be integral multiples of π). Assuming the X minimum is at the zone boundary ($k_0^X = 2\pi/a$), and the width of the barrier is L_B monolayers ($W = L_B a/2$), the propagation factor can be written as:

$$\begin{aligned} \exp(ikW) &= \exp(ik_0^X W)\exp(iqW) \\ &= (-1)^{L_B}\exp(iqW) \\ &= \begin{cases} +\exp(iqW), & \text{even } L_B \\ -\exp(iqW), & \text{odd } L_B \end{cases}. \end{aligned} \tag{3}$$

The L_B dependence of the X-channel conductance demonstrated in the equation above leads to the qualitatively distinct transmission spectra for even- and odd-L_B structures seen in Fig. 4, and ultimately is responsible for the radically different well-width dependences of Γ1 lifetimes seen in Fig. 2.

III. SUMMARY

We have studied the effect of Γ–X mixing on electron tunneling times in GaAs/AlAs symmetric double barrier heterostructures using an empirical tight-binding band structure model. We examined the hypothesis that X-point states provide additional channels for tunneling escape from the GaAs QW, and thereby shorten quasibound state lifetimes. However, our analysis indicates that both constructive and destructive interferences can occur between the Γ and X conductance channels in the AlAs barriers, and therefore the lifetime of the Γ1 quasibound state can either be lengthened or shortened by Γ–X mixing effects. Furthermore, because of the special properties of the X-valley tunneling states, we find that the Γ1 quasibound state lifetime is decreased or increased by Γ–X mixing depends on whether the AlAs barriers contain an even or odd number of monolayers.

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